Erratum: Nonlocal van der Waals functionals: The case of rare-gas dimers and solids (vol 138, 204103, 2013)

Tran, Fabien ; Hutter, Juerg

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Erratum: "Nonlocal van der Waals functionals: The case of rare-gas dimers and solids" [J. Chem. Phys. 138, 204103 (2013)]

Fabien Tran and Jürg Hutter
Institute of Physical Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

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Due to an error in the implementation of the exchange functional $C09_x$[1] in version 2.0.1 of LIBXC,[2] the results obtained with the $C09_x$-vdW functional reported in Tables II and III and Figs. 1–5 of Ref. 3 are wrong. The results obtained with the correct implementation of $C09_x$ are shown in Tables I and II. The main change in the conclusion is the overall better agreement with the reference results for the bond lengths R_0 of the dimers and lattice constants a_0 of the solids.

TABLE I. Equilibrium bond length R_0 (in Å) and interaction energy ΔE (in meV and with opposite sign) of rare-gas dimers calculated from the $C09_x$-vdW functional.

	He_2		Ne_2		Ar_2		Kr_2	
Functional	R_0	ΔE	R_0	ΔE	R_0	ΔE	R_0	ΔE
$C09_x$-vdW	3.11	3.8	3.32	7.4	4.05	14.6	4.33	18.0

TABLE II. Equilibrium lattice constant a_0 (in Å) and cohesive energy ΔE (in meV/atom and with opposite sign) of rare-gas solids calculated from the $C09_x$-vdW functional.

	Ne		Ar		Kr	
Functional	a_0	ΔE	a_0	ΔE	a_0	ΔE
$C09_x$-vdW	4.50	62	5.33	128	5.64	163

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[2] M. A. L. Marques, M. J. T. Oliveira, and T. Burnus, Comput. Phys. Commun. **183**, 2272 (2012).
[3] F. Tran and J. Hutter, J. Chem. Phys. **138**, 204103 (2013).

